Fluctuation formula for nonreversible dynamics in the thermostated Lorentz gas

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We investigate numerically the validity of the Gallavotti-Cohen fluctuation formula in the two and three dimensional periodic Lorentz gas subjected to constant electric and magnetic fields and thermostated by the Gaussian isokinetic thermostat. The magnetic field breaks the time reversal symmetry, and by choosing its orientation with respect to the lattice one can have either a generalized reversing symmetry or no reversibility at all. Our results indicate that the scaling property described by the fluctuation formula may be approximately valid for large fluctuations even in the absence of reversibility.

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The Lorentz gas (LG) thermostated by a Gaussian isokinetic (GIK) thermostat is one of the most popular models in the study of the relationship between transport properties and chaotic behaviour in nonlinear dynamical systems. Since the microscopic dynamics of the LG is chaotic, and on a sufficiently long time scales it possesses a well defined macroscopic transport coefficient, it can be used to study the connection of microscopic chaos and macroscopic nonequilibrium behaviour.

The so-called fluctuation formula (FF) has first been observed numerically in a system of thermostated fluid particles undergoing shear flow [1]. In that model, trajectory segments violating the second law of thermodynamics were found with probabilities exponentially smaller than those of trajectory segments associated with normal thermodynamical behaviour. More precisely, let $\xi_\tau(t)$ denote the *entropy production rate* ξ averaged over a time interval of length τ centered around time t: $\xi_\tau(t) = \frac{1}{\tau}\int_{-\tau/2}^{\tau/2} \xi(t+t')\,\mathrm{d}t'$, and let us consider it as a probabilistic variable. Then its statistical properties in a steady state can be characterized by a probability density $\Xi_\tau(x)$. The fluctuation formula states [2] that this probability density has the following property:

$$\lim_{\tau\to\infty} \frac{1}{\tau} \ln \frac{\Xi_\tau(x)}{\Xi_\tau(-x)} = x\,. \tag{1}$$

One of the interesting features of the FF is that it seems to be valid in systems far from equilibrium, not just for vanishing external fields.

After discovering the formula numerically, analytical results were obtained about its validity in deterministic systems like transitive Anosov systems [3] and special reversible maps [4, 5]. In the proofs of these theorems, the *time reversibility* of the system plays a key role [12]. Nevertheless, proving fluctuation theorems under more general conditions seems to be exceedingly difficult. In this context, even relatively simple systems like the LG, with or without magnetic field, seem to be out of reach for the existing analytical techniques. It is also unclear how the FF should look like in systems with nonreversible dynamics [6]. Consequently, reliable numerical results for such models may provide valuable hints in the search for more sophisticated theoretical approaches.

The field driven Lorentz gas consists of a charged particle subjected to an electric field moving in the lattice of elastic scatterers. For the sake of simplicity, we take a square or cubic lattice in our study, depending on the dimensionality of the system. Due to the applied electric field, one must use a thermostating mechanism to achieve a steady state in the system. Such a tool is the Gaussian isokinetic thermostat which preserves the kinetic energy of the particle; for a review see e.g. [7] and further references therein. We will also apply a constant external magentic field to control the reversibility of the dynamics.

Throughout our work we use dimensionless variables. We choose the units of mass and electric charge to be equal to the mass and electric charge of the particle, so we have $m = q = 1$ in our model. The unit of distance is taken to be equal to the radius of scatterers ($R = 1$), and the unit of time is chosen to normalize the magnitude of particle velocity to unity. Let $\mathbf{q} = (q_1, \ldots, q_n)$ denote the position and $\mathbf{p} = (p_1, \ldots, p_n)$ the momentum of the particle in the n-dimensional space ($n = 2$ or 3). Due to the normalization, $|\mathbf{p}| = 1$. The phase space variable of the system is $\mathbf{\Gamma} = (\mathbf{q}, \mathbf{p})$; it is transformed abruptly at every elastic collision and evolved smoothly by the differential equation

$$\begin{aligned} \dot{\mathbf{q}} &= \mathbf{p} \\ \dot{\mathbf{p}} &= \mathbf{E} + \mathbf{p}\times\mathbf{B} - \alpha\mathbf{p} \end{aligned} \tag{2}$$

between them. Here α is called the *thermostat variable*, while $\mathbf{E}$ and $\mathbf{B}$ are constant vectors playing the roles of the external electric and magnetic fields, respectively. The GIK thermostat corresponds to the choice $\alpha = \mathbf{E}\mathbf{p}$ in Eq. (2). For $n = 2$, $\mathbf{B}$ is thought to be perpendicular to the plane of motion given by the directions of $\mathbf{E}$ and $\mathbf{p}$. We note that Eq. (2) is dissipative, but for $\mathbf{B} = 0$ it has also time reversal symmetry.

Dissipation can be measured by the phase space con-

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traction rate σ. It can be computed by taking the divergence of the right-hand side of Eq. (2):

$$\sigma = -\mathrm{div}\,\dot{\mathbf{\Gamma}} = -\,(n-1)\,\alpha\,, \tag{3}$$

and it can be shown (see e.g. [8]) that in our case

$$\sigma(t) \;=\; \xi(t). \tag{4}$$

We note that the validity of this identity does depend on the choosen model and cannot be treated as a general property [7, 9, 10].

The notion of reversibility [11], an extension of time reversal symmetry, can be formulated in terms of the phase space flow $\mathbf{\Phi}^t$ defined by $\mathbf{\Gamma}(t) = \mathbf{\Phi}^t\mathbf{\Gamma}_0$. We say that the flow is reversible, if there exists a map $\mathbf{G}$ which is an involution (i.e $\mathbf{G}^2$ is the identity) and bracketing the flow by $\mathbf{G}$ reverses the direction of time:

$$\mathbf{G}\mathbf{\Phi}^t\mathbf{G} = \mathbf{\Phi}^{-t}. \tag{5}$$

Time reversal symmetry is a special case of reversibility with a particular choice of the involution: $\mathbf{G}_0(\mathbf{q},\mathbf{p}) = (\mathbf{q},-\mathbf{p})$.

In the LG, reversibility depends on the directions of the field vectors relative to each other and the lattice. It can be checked easily that our system is time reversible if $\mathbf{B} = \mathbf{0}$, and it is not otherwise. In Ref. [13], we have also shown that the system is still *reversible* for $\mathbf{B} \neq \mathbf{0}$ if the plane containing $\mathbf{E}$ and $\mathbf{B}$ is a symmetry plane of the lattice. Since the transformation $\mathbf{G} = \mathbf{M}\mathbf{G}_0$ (where $\mathbf{M}$ is a mirroring of $\mathbf{q}$ and $\mathbf{p}$ with respect to the plane containing $\mathbf{E}$ and $\mathbf{B}$) satisfies Eq. (5), the smooth flow is always reversible. This means that the reversibility of the full dynamics including the collisions requires that the invariant plane of $\mathbf{M}$ be a symmetry plane of the lattice [13]. In the two dimensional case this is simplified to the condition that $\mathbf{E}$ has to be contained by the symmetry plane of the lattice.

The goal of our numerical simulations was to measure $\Xi_\tau(x)$ with a precision which is sufficient to check the validity of the fluctuation formula. Due to Eq. (4), $\Xi_\tau(x)$ could be measured by periodically computing σ_τ along a particle trajectory and making a histogram of these data. The disadvantage of this method is that the range of possible σ_τ values depends on the strength of the electric field. Instead we may introduce the quantity

$$\pi_\tau(t) = \frac{1}{\tau}\int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} \mathbf{n}_{\mathbf{E}}\mathbf{p}(t+t^{'})\,\mathrm{d}t^{'}, \tag{6}$$

where $\mathbf{n}_{\mathbf{E}}$ denotes the unit vector paralell to $\mathbf{E}$. Since the magnitude of $\mathbf{p}$ is unity, π_τ always satisfies $\pi_\tau \in [-1,1]$. By making a histogram of the periodically measured values of π_τ, one gets an approximation of its probability density $\Pi_\tau(x)$. Since the two probabilistic variables satisfy $\sigma_\tau = (n-1)\,E\pi_\tau$, the connection of the probability densities is

$$\Xi_\tau(x) = \frac{1}{(n-1)E}\,\Pi_\tau\left(\frac{x}{(n-1)E}\right). \tag{7}$$

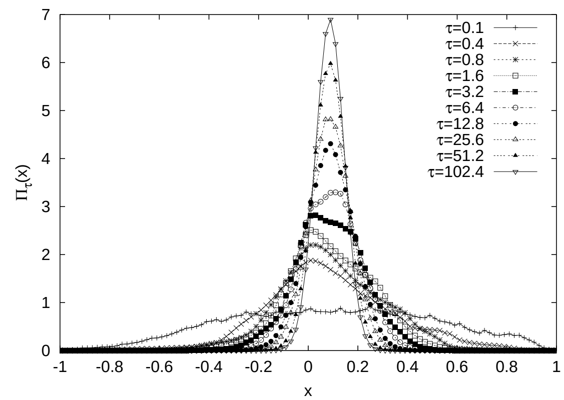

FIG. 1: The probability density $\Pi_\tau(x)$ for a 2D configuration, where $\mathbf{E} = (0.5, 0.8)$ and $|\mathbf{B}| = 0.2$. The distance between the centers of the scatterers is $d = 2.1$; the number of collisions is 1.6×10^8, while the average time between two collisions is ≈ 0.6. These data are similar throughout all examples presented in this paper.

Then we can rewrite the fluctuation formula as

$$\lim_{\tau\to\infty} \frac{1}{(n-1)E}\frac{1}{\tau}\,\ln\frac{\Pi_\tau(x)}{\Pi_\tau(-x)} = x\,. \tag{8}$$

At a first glance, $\Pi_\tau(x)$ behaves similarly in all cases: as τ grows, $\Pi_\tau(x)$ becomes more and more concentrated around its mean value. This typical shape is shown in Fig. 1. It can be noticed that the curve looks like a Gaussian, although it is clear that it must be different due to the finite range of x [14]. In a separate paper [15], we will deal with the properties of this distribution in more details. In order to visualize the fluctuation formula, we introduce the quantity

$$D_\tau(x) = \frac{1}{(n-1)E}\frac{1}{\tau}\,\ln\frac{\Pi_\tau(x)}{\Pi_\tau(-x)} \tag{9}$$

that must exactly be linear with a slope 1 in the $\tau \to \infty$ limit if the fluctuation formula is valid. We will investigate for different configurations of the LG how well $D_\tau(x)$ approaches this behavior in numerical simulations. Due to the fact that we have a finite number of data points coming from a numerical trajectory of finite length, our conclusions concerning $D_\tau(x)$ and thus the fluctuation formula are, of course, limited to an interval $[-\Delta_\tau, \Delta_\tau]$ with $\Delta_\tau \leq 1$. In practice, if the extremal π_τ values in a series of N measured data were π_{min} and π_{max}, then we identified Δ_τ with $\min(-\pi_{min}, \pi_{max})$. It is easy to check that the probability of observing π_τ values outside this interval in another series is in the order of $1/N$. Fig. 2 shows the τ dependence of Δ_τ for different field strengths with N fixed. For our simulations, N was chosen to be 10^9, which means that if $D_\tau(x)$ is found to be linear on $[-\Delta_\tau, \Delta_\tau]$ with slope 1, then it can be interpreted as the fluctuation formula is valid for fluctuations with probabilities larger than 10^{-9}.

In the rest of the paper, we present our numerical results for the GIK thermostatted LG both in two and three

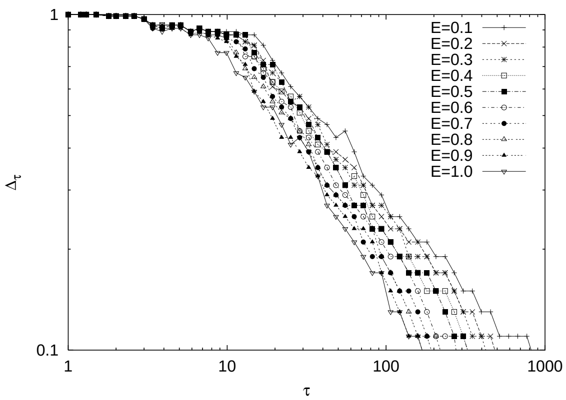

FIG. 2: The dependence of Δ_τ on τ for different field strengths in a 2D configuration with $\mathbf{B} = 0$. The direction of $\mathbf{E}$ is parallel with $(5, 8)$ but its magnitude varies. The curves appear to be linear in the dominant region on the log-log plot, suggesting a power law dependence on τ. This behavior seems to be valid for other configurations as well, no matter they are reversible or not.

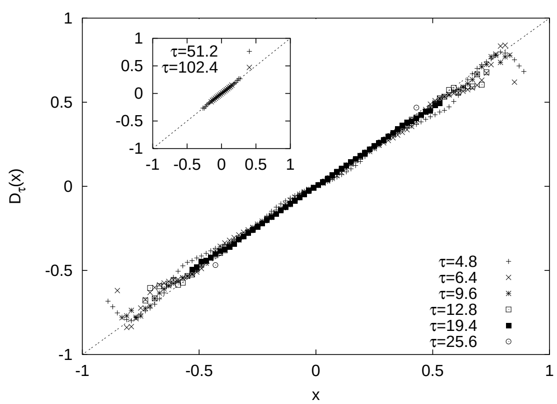

FIG. 3: $D_\tau(x)$ for a time reversible configuration ($\mathbf{B} = 0$) in 2D with $\mathbf{E} = (0.5, 0.8)$. The inset shows that for higher τ values, $D_\tau(x) \approx x$ on $[-\Delta_\tau, \Delta_\tau]$. The inset has the same axes as the figure.

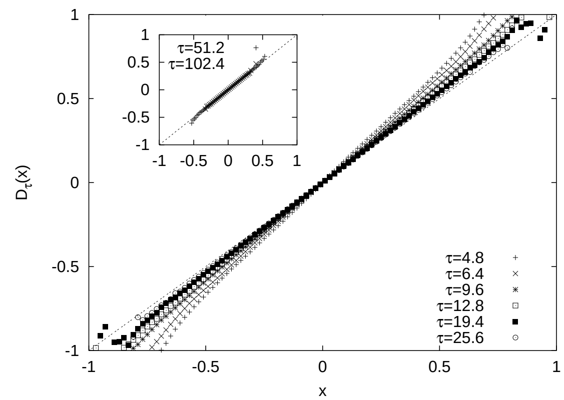

FIG. 4: $D_\tau(x)$ for a time reversible configuration in 3D, with $\mathbf{E} = (0.05, 0.1, 0.15)$ and $\mathbf{B} = \mathbf{0}$. The inset shows that $D_\tau(x)$ converge to x as τ gets larger. The axes of the inset are the same as in the figure.

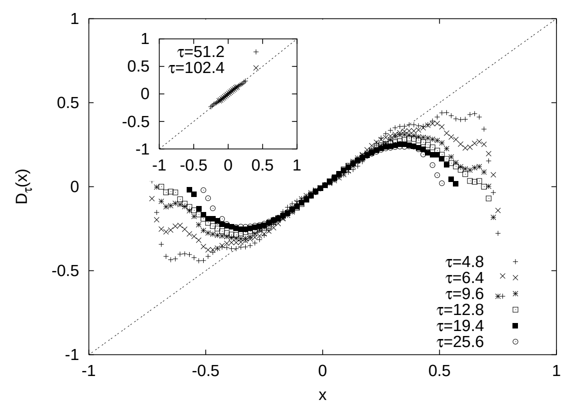

FIG. 5: $D_\tau(x)$ for a nonreversible configuration in 2D, with $|\mathbf{B}| = 0.2$ and $\mathbf{E} = (0.5, 0.8)$. It seems that for lower τ values $D_\tau(x)$ has a breakoff from the linear curve around $x \approx \pm 0.3$, but the inset shows that for higher τ values, $D_\tau(x)$ behaves quite similarly to the reversible case of Fig. 3. We note that this is the same configuration as the one used for Fig. 1. The inset has the same axes as the figure.

dimensions, with various values of the external fields. We focus on the question whether nonreversible dynamics leads to different scaling in the fluctuations than the one found in reversible systems. As a general rule, we have not found any difference between time reversal symmetric cases (i.e., with $\mathbf{B} = 0$) and reversible ones. Indeed, time reversal symmetry can be replaced in the known fluctuation theorems by general reversibility without affecting their validity, since the proofs do not make use of the special form of the involution $\mathbf{G}_0$. We note that we have tested the different dynamical cases with several choices for the field stregths and could not find significant deviations in the observed behavior as long as we stayed within the ergodic region of the parameter space.

In Figs. 3 and 4, we plot $D_\tau(x)$ for reversible dynamics in two and three dimensions (2D and 3D), respectively. The fluctuation formula appears to be valid in both cases; the convergence to the linear limit, however, seems to be different in them. For 2D, the $D_\tau(x)$ curve has deviations, decreasing in size with τ increasing, from the linear shape, while for 3D, $D_\tau(x)$ exhibits strongly linear behavior with slopes approaching 1 as τ increases. It is worth noting that the latter convergence can also be observed in the 2D *random* LG [16].

Our results for the nonreversible versions are shown in Figs. 5 and 6. The most striking difference compared to the reversible cases is the fact that there seems to be a *cubic* term present in $D_\tau(x)$ that does not disappear for larger τ values. This term leads to a breakoff from the diagonal line for $|x| \geq x_c \approx 0.3$, which means that there can be deviations from the fluctuation formula for *large* fluctuations. The slope of the linear part, however, is still 1 in the large τ limit, so the FF can be a good approximation for small to moderate size fluctu-

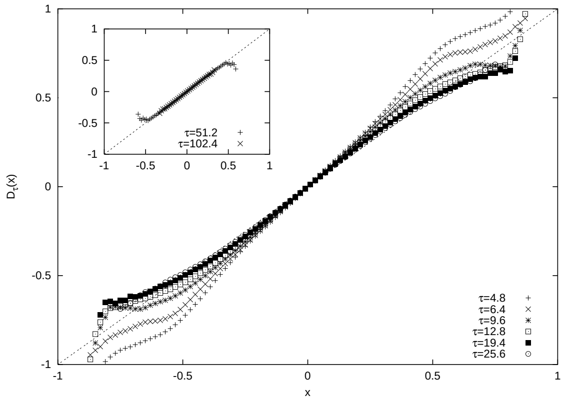

FIG. 6: $D_\tau(x)$ for a nonreversible configuration in 3D, with $\mathbf{E} = (0.05, 0.1, 0.15)$ and $\mathbf{B} = (0.16, -0.06, 0.04)$. The axes of the inset are the same as in the figure.

ations. The fact that the region of validity of the FF does not shrink considerably for larger τ values suggests that the coefficient of the cubic term in $D_\tau(x)$ may have only weak dependence on τ. This also means that as the distribution $\Pi_\tau(x)$ is concentrating around its mean value for increasing τ values, the total statistical weight of the large fluctuations that are not covered by the linear regime is decreasing. In other words, the FF becomes more and more valid in a probabilistic sense as $\tau \to \infty$, since the larger fluctuations become less and less likely in that limit.

We may conclude that the FF appears to be valid in the GIK thermostated LG with reversible dynamics, both in two and three dimensions. For nonreversible dynamics, we have found indications that the FF may still describe the scaling properties of fluctuations in a moderate size regime, although for large fluctuations there are clear deviations from it due to higher order terms in $D_\tau(x)$. The fact that the slope of the linear part in the scaling behavior is the same in reversible and nonreversible cases suggests a kind of robustness for the FF in the thermostated LG. It would be interesting to see if this remains valid in other nonequlibrium systems with nonreversible dynamics.

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